

## II.2. Simple Concepts of Classical Mechanics

In the following, simple *mechanical concepts of energy and equilibrium* are recapitulated, emphasizing what will be used in later discussion of thermodynamic theory. In addition, illustrations of simple dynamics will be given. They will become useful in applications of kinetic theory and partition functions. Classical concepts, which are often used in physical chemistry, include different forms of *energy*, interaction *force*, etc. They will be mentioned here without in-depth analysis, which is delegated to individual review of texts on theoretical mechanics.

A *force*  $F$  acting on an object (particle) of *inertia* (mass)  $m$  tends to either repel or attract it, from or to, respectively, some region in space, depending on its character. For simplicity, first objects are considered that can move only along a *single spatial degree of freedom*, say  $x$ . For unbound objects, this force leads to an *acceleration*  $a$ , the rate  $a = dv/dt$  of temporal change of the relative velocity  $v$ , given by

$$F = m \ddot{x} a \quad (\text{II.32})$$

which is called *Newton's Law*. Since the *linear momentum* is defined by  $p = m \dot{x} v$ , Equ. II.32 is equivalent to

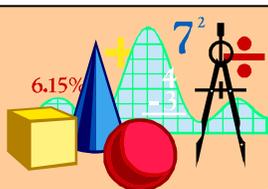
$$F = \frac{dp}{dt} = \dot{p} \quad (\text{II.33})$$

To move a body a distance  $d$  against the resistance of a constant force  $F \eta \text{ const.}$ , e.g., one due to a linear electric field tending to push a charged object (particle) the other way, requires the *energy*

$$E = F \int dx d \quad (\text{II.34})$$

If the situation is characterized by a variable force,  $F = F(x)$ , i.e., a non-linear energy field, the *energy  $\Delta E$  gained by a body* moving in the force field from point  $x_0$  to point  $x$  is given by the integral

$$\Delta E(x, x_0) = \int_{x_0}^x dx' F(x') = \int_{x_0}^x dE(x') = E(x) - E(x_0) \quad (\text{II.35})$$



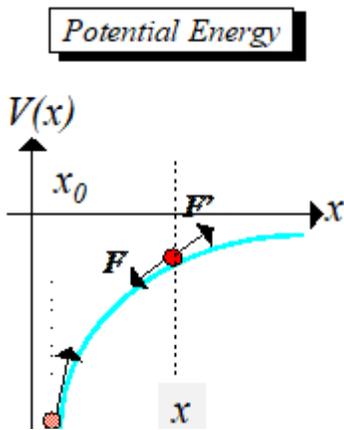
*A few mathematical remarks:* Note that the *variable  $x'$  of the integrand* (under the integral sign) in Equ. II.21 must be different from the *integral limits*, which are specific values of this variable ( $x' = x_0$  and  $x' = x$  in this example). The function

$$dE(x') = \frac{\partial E}{\partial x'} \cdot dx' = F(x') \cdot dx'$$

is the *exact differential of the function  $E(x')$* ,  $E$  is the *primitive function (“integral”) of  $dE$* . The value of the above integral is given completely by just the difference in two numbers, the values of the energy at two positions ( $x_0$  and  $x$ ) of the body. It does not matter, on which particular path the body came from  $x_0$  to  $x$ .  $E$  is a *state function*. Later on, integrals of *inexact differential* will be discussed, where the value of the integral does depend on this path.

If an unbound particle of mass  $m$  is accelerated by a force  $F$  over a distance ( $x_0 \rightarrow x$ ), the associated energy is converted entirely into additional kinetic energy  $\Delta E_{kin}$  of the particle,

$$\Delta E_{kin} = \Delta E(x, x_0) = \frac{1}{2} m [v^2(x) - v^2(x_0)] \quad (\text{II.36})$$



**Figure II-25**

If, on the other hand, the particle is bound such as, e.g., a particle resting on the bottom of a potential (gravitational) well would be, it requires a force  $F'(x) > -F(x)$  overcompensating the force  $F(x)$  due to the potential, in order to raise the particle to a level of higher *potential energy*

$$\Delta E_p = V(x) - V(x_0) = - \int_{x_0}^x dx' F(x') \quad (\text{II.37})$$

The force  $F'(x) = -F(x) > 0$  counteracts exactly (“balances”) the binding force  $F(x) < 0$  representing the action of the potential. In this case, one speaks of a *static equilibrium of forces*, leaving the particle motionless, at exactly the same height. The binding force has a *negative sign, if it attracts the particle into the region of smaller x values*. One describes the process of lifting the particle against the resistance by the potential as *work (w) done against an external force*

$$F = - \frac{\partial \mathcal{N}}{\partial x} \quad (\text{II.38})$$

associated with the *driving potential*. The lifted body has gained *potential energy equal to the work done*,  $w = \Delta E_p$ . The entity

$\partial V / \partial x$  is the *partial derivative of  $V$  with respect to  $x$* , keeping all other variables fixed, except  $x$ .

In three spatial dimensions, with a position vector  $\vec{r} = (x, y, z)$  expressed in terms of Cartesian coordinates  $x$ ,  $y$ , and  $z$ , this is generalized to:

$$\vec{F} = -\text{grad } V(\vec{r}) = -\vec{\nabla}V(\vec{r}) = -\left\{ \frac{\partial V}{\partial x} \vec{u}_x + \frac{\partial V}{\partial y} \vec{u}_y + \frac{\partial V}{\partial z} \vec{u}_z \right\} \quad (\text{II.39})$$

where the  $\vec{u}_i$  ( $i=x,y,z$ ) are *unit vectors in the respective directions*. The vector operator  $\vec{\nabla}$  is called "*del*" or "*nabla*" operator. The equation

$$\dot{\vec{p}} = \vec{F} = -\text{grad } V(\vec{r}) \quad (\text{II.40})$$

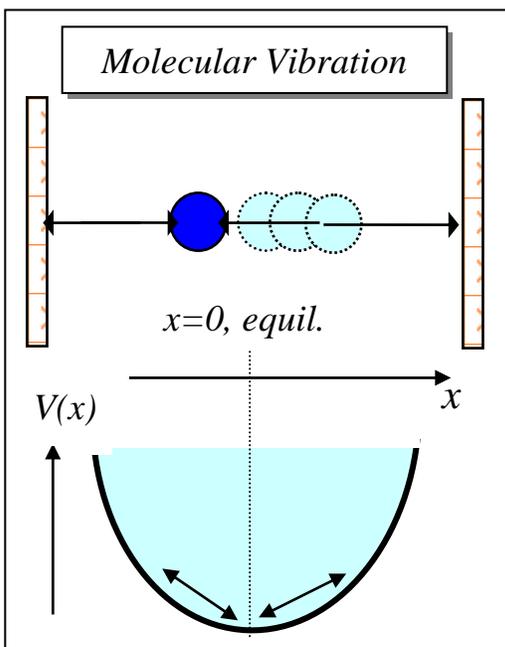


Figure II-26

then results as the *fundamental EOM (equation of motion)* of the Newtonian mechanics.

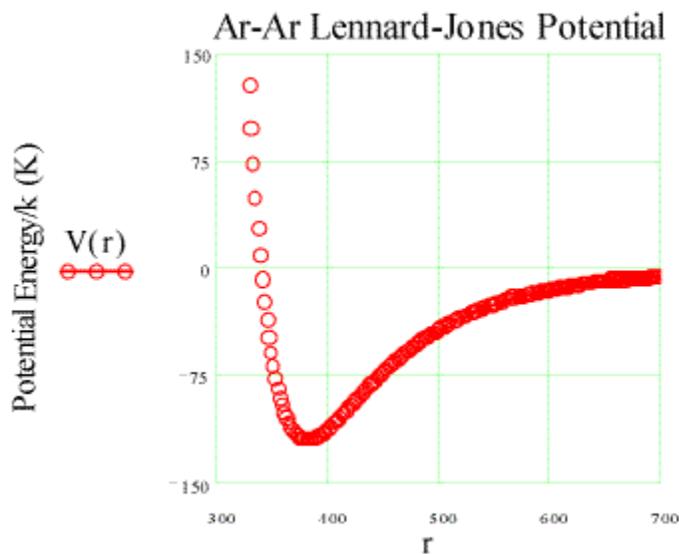
This equation is illustrated in Fig. II-26 for the simple case of a *Harmonic Oscillator* representing, e.g., a vibrating atom in a linear molecule (bond-stretching mode). For simplicity, one replaces the atoms on the left and right by rigid walls, such as shown in the sketch. This is a simplification, since the adjacent molecules may also vibrate and exert an external force on the atom. To illustrate the accuracy of the

harmonic-oscillator approximation, consider an actual interaction potential  $V(r)$  for the interaction between two  $Ar$  atoms at distance  $r$  from each other. The potential is well described by the **Lennard-Jones** form

$$V(r) = 4\varepsilon \cdot \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (\text{II.41})$$

with a strength parameter, given relative to the Boltzmann constant as  $\varepsilon/k_B = 120 \text{ K}$ , and a range parameter of  $\sigma = 341 \text{ pm}$  [ $1 \text{ pm} = 1 \times 10^{-12} \text{ m}$ ]. The corresponding force is calculated as

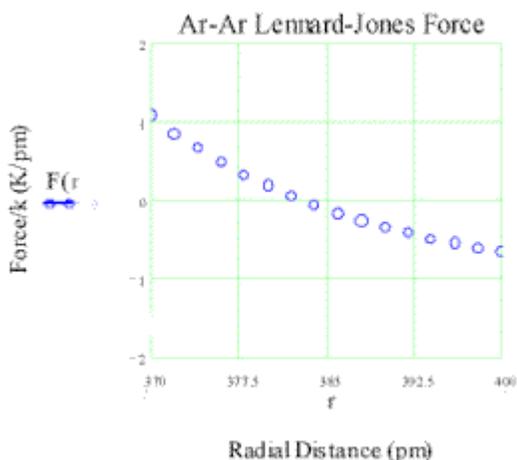
$$F(r) = -\frac{dV}{dr} = \frac{24}{\sigma} \varepsilon \cdot \left[ 2 \left( \frac{\sigma}{r} \right)^{13} - \left( \frac{\sigma}{r} \right)^7 \right] \quad (\text{II.42})$$



**Figure II-27** Radial Distance (pm). One observes from Fig. II-27 that the potential has a **repulsive core at small distances**, a minimum, and a shallower **attractive negative part at longer range** ("tail"). Figure II-28 shows, that the corresponding force goes through zero, at approximately  $r = r_{eq} \approx 382.5 \text{ pm}$ . This

The above  $Ar$ - $Ar$  interaction energies and forces are plotted in Figs. II-27 and 28 vs. the distance  $r$  between the  $Ar$  atoms (note the slightly different  $r$  scales!). The calculation use the code [MATHCAD 252\ArAr\\_LJ\\_Inter.mcd](#).

One observes from Fig. II-27 that the potential has a **repulsive core at small distances**, a minimum, and a shallower **attractive negative part at longer range** ("tail").

**Figure II-28**

*potential, i.e., an attractive, long-range part and a repulsive short-range core. Of course, the energy scales are different and characteristic of the associate length scales of the interacting objects.*

If the interaction potential had an approximately quadratic  $r$ -dependence, then the force would be exactly linear in  $r$ . This is obviously not quite the case. The force is approximately linear only in a range of  $\pm 5$  pm about the equilibrium point of the potential. Hence, only very small oscillations about the equilibrium may actually be considered harmonic.

The harmonic approximation consists in a *restriction to only very small oscillations* about the equilibrium position  $\mathbf{x} = (\mathbf{r} - \mathbf{r}_{eq}) = \mathbf{0}$ . Then, the *restoring force* in  $x$ -direction is *approximately linear* and given by *Hooke's Law*

$$F = -c\mathbf{x}$$

(II.43)

zero demarcates the *equilibrium point of the potential*, the bottom of the potential. At this "bond distance", no net force acts on the atoms, which are attracted to each other at larger distances and repelled at smaller ones.

*It is interesting to note that the potential describing the interactions between so different entities as atoms, nuclei, and nucleons, have qualitatively the shape of a Lennard-Jones*

Here,  $c > 0$  is the restoring-force constant, and the sign of  $F$  indicates the direction of its action. The associated *harmonic-oscillator potential* is given by

$$V(x) = (1/2)c\exists x^2 \quad (\text{II.44})$$

It is easy to verify that the negative gradient of this potential is indeed equal to Hooke's force. The magnitude of the force constant  $c$  can be obtained from a fit of the approximation of Equ. II.44 to the actual potential, which may be of the type of Equ. II.41.

With the momentum of the vibrating atom given by  $p = m\dot{x}$ , the equation of motion reads:

$$\frac{dp(t)}{dt} = F = -cx(t) \quad \text{or} \quad m\ddot{x}(t) = -cx(t) \quad (\text{II.45})$$

In this *linear regime*, the *vibrator must behave orderly*, the motion is cyclic. Consequently, these equations have the oscillatory solutions

$$x(t) = x(t=0)\exists \cos(\omega t) \quad (\text{II.46a})$$

or

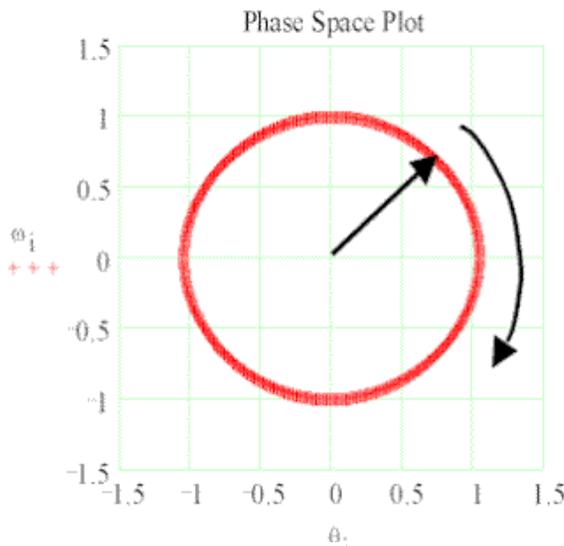
$$x(t) = x(t=0)\exists \sin(\omega t) \quad (\text{II.46b})$$

with an *amplitude*  $x(t=0)$  and an oscillatory factor depending on the *circular frequency*

$$\varpi = \frac{2\pi}{T} = \sqrt{\frac{c}{m}} \quad (\text{II.47})$$

This frequency is related to the *period  $T$  of the oscillatory motion* by  $\omega = 2\pi/T$ . Obviously, for times  $t_n = nT$  ( $n=0,1,2,\dots$ ) the

*phase of the sine (or cosine) function* is an integer multiple of  $2\pi$ ,



$x(t_{n-1}) = x(t_{n-2}) = x(t_{n-3}) = \dots = x(t_{n-4}) = \dots$  = f cyclic motion with the cycle

the larger Hooke's constant is and the vibrating object, the higher its frequency.

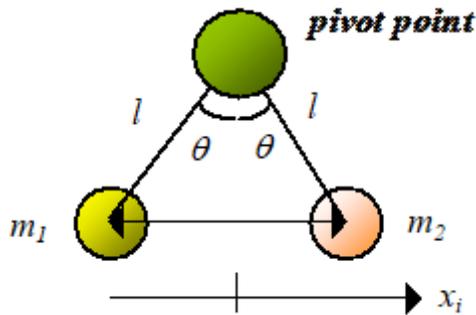
Equ. II.46 should be adopted describing the system at  $t = 0$ . For example, if the mass is at its maximum  $x(0) = x_0$  on the

the **Figure II-29** where the atom reverses its velocity, then the appropriate solution would be

$$x(t) = x_0 \cdot \cos(\omega t)$$

**Molecular Bending Vibration**

$$\dot{x}(t) = -x_0 \omega \cdot \sin(\omega t) \quad (\text{II.48})$$



Equ. II.48 is for the  $t$ -dependence of the velocity (or momentum) are correlated with the same period  $T$ , but by  $90^\circ$  represented in a *phase (space) diagram*, prescribes an elliptic orbit

**Figure II-30**

velocity vs. angular position. Plotting the normalized velocity vs. position, e.g.,  $\dot{x}(t)/x_0\omega$  vs.  $x(t)/x_0$ , one obtains a unit circle.

Oscillator dynamics are a feature occurring for many molecules, as is illustrated in a simple example of molecular bending-mode vibrations. This could be, for example, an  $H_2O$  molecule or per-

haps a subcluster of a larger molecule. The atoms of masses  $m_1$  and  $m_2$  ( $= m_1 = m$ , for simplicity) are placed in the  $t$ -dependent geometry of an *equilateral triangle of fixed side length  $l$* , where they can pivot about the point (center atom) at the top of that triangle, changing the distance  $x = x_2 - x_1$  between the two atoms. If the atom-atom interaction is of a *van der Waals (Lenard-Jones)* type, then there is an equilibrium distance  $x = x_{equ}$  between the two atoms, i.e., there is attraction for larger and repulsion for smaller distances.

Assume for simplicity then the linear force law of the type of Equ. II.43,  $F = -c\mathfrak{E}(x - x_{equ})$ , where  $x_{equ}$  is the equilibrium distance between the atoms and  $c > 0$  the *restoring-force constant*. This problem is really one of rotational motion of the atoms at a fixed radius  $r = l$  about the pivot point, with the only degree of freedom being the *bond angle  $2\theta$* . Then, the problem is solved easiest when expressed in that coordinate. First, the force *acting between the two atoms 1 and 2* is written in terms of half the bond angle,  $\theta = (\theta_1 + \theta_2)/2$ :

$$F = -c\mathfrak{E}\mathfrak{E}(\sin\theta - \sin\theta_{equ}) \quad (\text{II.49})$$

For *small deviations about the equilibrium*, where  $\sin\theta - \sin\theta_{equ} \approx \theta - \theta_{equ}$ , one recovers essentially the force law for (rotational) harmonic oscillations ([Equ. II.43](#)) about the equilibrium bond angle of  $2\theta = 2\theta_{equ}$  with a modified force constant. This approximation is used here for illustrative purposes, but is not made in the numerical calculations explained further below.

It is important to realize that the above force accelerates the two atoms relatively to one another, it acts on the *relative motion of the two interacting atoms*. The total kinetic energy of this rotation is the sum of the individual kinetic energies

$$K = K_1 + K_2 = \frac{m_1}{2} v_1^2 + \frac{m_2}{2} v_2^2 = \frac{1}{2} \left[ m_1 (\ell \dot{\theta}_1)^2 + m_2 (\ell \dot{\theta}_2)^2 \right] \quad (\text{II.50})$$

For equal masses,  $m_1 = m_2 = m$  as assumed here, this expression simplifies considerably:

$$K = \frac{1}{2} \left[ m_1 (\ell \dot{\theta}_1)^2 + m_2 (\ell \dot{\theta}_2)^2 \right] = \frac{m}{2} \ell^2 \dot{\theta}_1^2 + \dot{\theta}_2^2 \quad (\text{II.51})$$

Since both atoms move each with the same individual velocity either towards the other or away from it, i.e.,  $\dot{\theta}_1 = -\dot{\theta}_2 = \dot{\theta} = \omega$  the relative velocity between the two atoms is given by

$$\begin{aligned} v_{rel} &= \frac{d}{dt} (\ell \sin \theta_1 - \ell \sin \theta_2) = \ell \cos(\theta) (\dot{\theta}_1 - \dot{\theta}_2) \\ &= 2\ell \cos(\theta) \cdot \dot{\theta} = 2\ell \cos(\theta) \cdot \omega \end{aligned} \quad (\text{II.52})$$

Here, a popular assumption of  $\cos(\theta) \approx 1$  would actually not be very good. In terms of this relative velocity, the kinetic energy of bending is

$$K = \frac{m}{2} 2(\ell \cdot \cos(\theta) \cdot \omega)^2 = \frac{m}{2} \cdot \frac{v_{rel}^2}{2} = \frac{\mu}{2} v_{rel}^2 \quad (\text{II.53})$$

This equation has been derived for this particular case equal masses. However, it enjoys in fact a much more general validity. For the *relative motion of two bodies*, the *reduced mass*

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \quad (\text{II.54})$$

is the characteristic mass, and the *relative velocity*  $v_{rel} = v_1 - v_2$  is the characteristic velocity. *For the case of equal masses, the reduced mass is equal to half the mass of each particle,  $\mu = m/2$ .*

It is this fictitious particle that is accelerated by the force  $F$  to an increased (relative) velocity, corresponding, in the present example, to a temporal rate of change of the relative angle between the two atoms, which is equal to the total bond angle. As an equation for the present bending motion, one obtains

$$\frac{dp}{dt} = \frac{d(\mu v_{rel})}{dt} = \frac{d(\mu 2\ell \varpi \cos \theta)}{dt} = F = -c 2\ell (\sin \theta - \sin \theta_{equ}) \quad (\text{II.55})$$

In the small-amplitude approximation,  $\theta \approx \theta_{equ}$  and

*In general, one can represent the relative motion of two particles with respect to one another by that of a fictitious particle with a mass equal to the reduced mass  $\mu$ , moving with a velocity given by the relative velocity  $v_{rel}$ .*

$\sin \theta - \sin \theta_{equ} \approx \cos \theta_{equ} (\theta - \theta_{equ})$ , the above equation reduces to one of the type of [Equ. II.45](#) for harmonic oscillations of the bond angle:

$$\frac{d^2(\theta - \theta_{equ})}{dt^2} = \ddot{\theta}_1 = -\ddot{\theta}_2 = \frac{d\varpi}{dt} = \frac{F}{2\mu\ell} = -\frac{c}{\mu} (\theta - \theta_{equ})$$

While the approximate Equ. II.56 has obviously simple analytical solutions, the more accurate differential equation II.55 is slightly more difficult to solve. The solution of this latter equation presents an opportunity to apply *numerical integration methods* (see [Tutorial](#)), which are useful in many different areas of physics and

chemistry. They allow one to treat much more complicated problems than one can hope to solve analytically.

The equation of motion II.56 is solved here numerically to simulate the symmetric bending vibrations of the  $H_2O$  molecule, using the [Euler-Cromer](#) method for the integration of the differential equation. It suffices to know the experimental vibrational frequency  $\bar{\nu}_0 = 1595\text{ cm}^{-1}$  and the equilibrium bond angle  $\theta_{equ} = 104.5^\circ$  of the  $H_2O$  molecule to perform the simulation calculations, which has been done with the *MATHCAD* program [MATHCAD\\_252\Bending\\_VibesN.mcd](#). The results can be viewed as an [animation](#) showing regular harmonic oscillations about the equilibrium bond angle. The [phase diagram](#) is, as expected from the character of the solutions [compare [Eqs.II.46](#)] a closed ellipsis.

One of the great advantages of numerical simulation calculations is the ease by which additional physical phenomena can be accounted for. For example, if the above water molecules are not in free space but interact with other particles, e.g., those of a host vapor or gas, the  $H_2O$  bending vibrations will be slowed down by frictional forces. As will be shown in a later section, *random collisions between the molecule and vapor particles* which are in thermal motion lead to classical *friction forces* that are proportional to the velocity  $\dot{\theta}$  of the molecule,

$$F_{frict} = -\gamma \dot{\theta} \quad (\text{II.57})$$

Here,  $\gamma > 0$  is a frictional strength parameter. The negative sign is necessary to account for the slowing-down action of this force: it decelerates. Frictional or viscosity parameters are known experi-

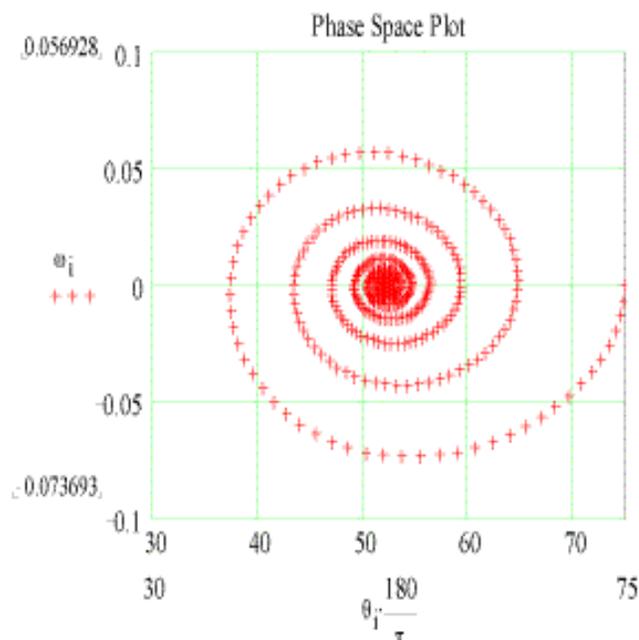
mentally for many gases and liquids. Frictional forces can simply be added to the conservative [Lennard-Jones force](#)  $F$  in Equ. II.56.

Another effect that may possibly influence the motion of  $H_2O$  molecules is due to its coupling to other molecules which also vibrate, but with frequencies  $\omega_D$  characteristic of their own normal modes. They could exert an external driving force  $F_D$  on the  $H_2O$  molecule. The molecule could also be subjected to an oscillating external electric field. In both cases, the  $H_2O$  molecule would feel a driving force of the type

$$F_D(t) = F_D \cdot \sin(\omega_D t) \quad (\text{II.58})$$

which again can be added simply to the force in Equ. II.56.

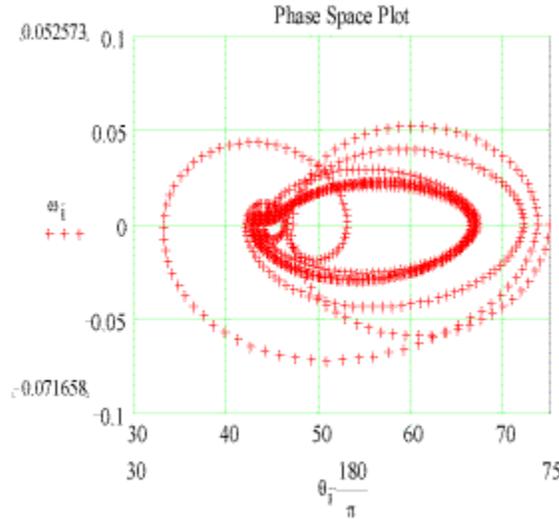
Both of the above effects are modeled in the *MATHCAD* code [MATHCAD\\_252\Bending\\_VibesN.mcd](#). The effect of a moderately strong friction force ( $\gamma=0.04$ ) can be seen directly in the [animation](#). The phase space plot for a damped vibrator is shown in Fig. II-31.



**Figure II-31: Phase plot for damped bending vibrations**

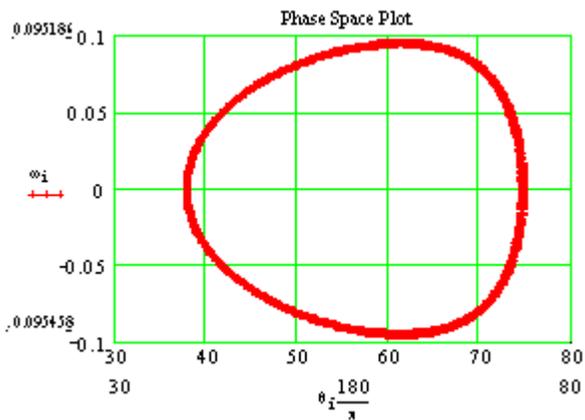
As is obvious from this plot, the bending motion is no longer strictly cyclic. The oscillations are damped, leading to *a spiral phase space plot* indicating a decrease of both position and velocity amplitudes, as time proceeds. Eventually, the bending vibrations subside completely, the molecule remains in its equilibrium state. Quantum-mechanically, of course, there would still *be zero-point oscillations*.

With the presence of an additional external driving force  $F_D$ , the bending motion becomes more complex. As an example, the [animation](#) illustrates the erratic behavior of the  $H_2O$  molecule, when it is subjected to a moderately strong external force ( $F_D=0.009$ ) with a frequency  $\omega_D = 1/3 \omega_0$ , one-third of that of the  $H_2O$  bending mode. Although not cyclic, the motion is not completely chaotic, either. The phase plot shows interesting pirouettes leading eventually to a quasi-stable orbit. The corresponding feature in the phase space plot is an approximate ellipse, the so-called *limit-circle*. It appears somewhat broad, because it is only roughly outlined by the trajectory which fluctuates somewhat about the average.



**Figure II-32: Bending vibrations with external excitation**

The above calculations have assumed small oscillations about the equilibrium bond angle, for which  $\sin \theta \approx \sin \theta_{eq}$  and



**Figure II-33**

$d(\sin \theta)/dt \approx d\theta/dt$ . Therefore, the above results for forced vibrations cannot be taken too literally. However, to make such approximations is not necessary in numerical calculations, which can easily be modified. Taking the full expression for  $\ddot{\theta}$  corresponding to Equ. II.55 (see homework problem), instead of the

approximate Equ. II.46, leads ([MATHCAD 252\Bending\\_VibesEx.mcd](#)) again to the same classes of orbits as before in the approximate calculations. Now, however, the oscillations are no longer of the pure sine or cosine types. Correspondingly, the closed orbits in the  $\omega$ - $\theta$  phase plane are no

longer ellipses or circles but have a pear-like shape, as seen in the figure. This is due to the fact that the distance between the atoms changes more rapidly at smaller than at larger bending angles, a reflection of the sine-dependence of this distance. The behavior for damped and forced oscillations modifies accordingly.

The phase plot below illustrates a trajectory for  $H_2O$  bending vibrations with moderate friction ( $\gamma = 0.02$ ) and moderate ( $F_D=0.009$ ) driving forces. The trajectory makes loops and pirouettes, before it settles down on a quasi-stable orbit. The final orbit is qualitatively *bi-stable*: it oscillates erratically back and forth between the two regions in angle about  $45^\circ$  and  $60^\circ$ , which are the *attractors* of the vibrator. The vibrational trajectory, which in other examples discussed above had a smooth behavior, following basically the same general sense, has *bifurcated*. The richness of the motion that such a simple system can exhibit for different combinations of the various forces, is quite intriguing. It is discussed in detail in dedicated studies of [chaotic dynamics or deterministic chaos](#).

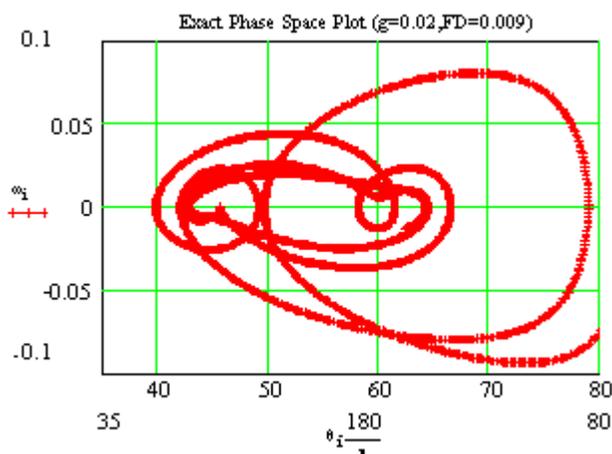


Figure II-34

Depending on the relation between the strength of the frictional and driving forces, the vibrational motion can degenerate to a completely chaotic vibration filling an entire region of the phase space almost uniformly. Such *completely chaotic systems visit essentially each point in phase space in time*, if one waits long enough. Therefore,

for completely chaotic motion, no point in phase space is preferred

over another. This is the *Principle of Equal A Priori Probability*, a postulate that is of fundamental importance for statistical thermodynamics.

## *Summary and Appendix II.2*

In this section, simple concepts of mechanics that are of importance for the understanding of the behavior of chemical systems have been discussed. They include the concept of a *force* and its relation to the conservative *potential*. A body is in *mechanical equilibrium*, if all applied forces balance out to zero, leaving the body at rest or in a state of steady motion. Force acting over a distance imparts energy on a particle. *Newton's Law*, relating the force to a temporal change of an object's linear momentum, provides a differential *equation of motion* for that object.

Linear force laws lead to oscillatory motion such as the symmetric bending vibrations of an  $H_2O$  molecule. The motion of two particles can be described efficiently in terms of a fictitious particle with a mass equal to the *reduced mass* of the particles, moving with a velocity equal to the *relative velocity* of the two particles. The *system trajectories* can be pictured in a *phase plot*, where oscillatory motion leads to elliptic closed orbits. *Nonlinear forces* lead to a complex, even *chaotic*, behavior of simple mechanical systems. Simulations of the motion can be performed with *numerical*, iterative *integration* of the differential equations defining the system trajectories.

### **Further Reading:**

S.E. Koonin, *Computational Physics*, Benjamin/Cummings (Menlo Park), 1986

R.H. Landau and M.J. Paez, *Computational Physics*, John Wiley & Sons (New York), 1997

N.J. Giordano, *Computational Physics*, Prentice Hall (Upper Saddle River, N.J.) 1997

## ***Appendix II.2: MATHCAD Programs and Tutorials***

The following Tutorials are called in the *Interactive Lecture/Study Notes* for Section II.1.6, when the corresponding links are activated.

### [Complex Numbers.doc](#)

Summarizes representations of and calculations with complex numbers.

### [Int\\_DiffEOM.doc](#)

Numerical methods for integrating differential equations of motion.

### [Taylor Expansion.doc](#)

Successive series approximation of a function at a given point, based on the derivatives.

The following *MATHCAD* programs are called in the *Interactive Lecture/Study Notes* for Section II.1.6, when the corresponding links are activated.

### [MATHCAD 252\ArAr LJ Inter.mcd](#)

Calculation of the Lennard-Jones interaction potential and force for Ar-Ar interactions

### [MATHCAD 252\DmpdOscill.mcd](#)

Calculates the motion of a damped oscillator and produces plots of position and velocity, also as phase space plots

### [MATHCAD 252\Bending Vibes.mcd](#)

Performs numerical integration of small-amplitude bending vibrations of the  $H_2O$  molecule, including damping and external driving forces.

[MATHCAD\\_252\Bend\\_Vibs.avi](#)

Video clip of regular  $H_2O$  bending vibrations

[MATHCAD\\_252\Bend\\_Vibs\\_dmd.avi](#)

Video clip of damped  $H_2O$  bending vibrations

[MATHCAD\\_252\Bend\\_Vibs\\_caos.avi](#)

Video clip of chaotic, driven  $H_2O$  bending vibrations